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Correlation between diffusion and coherence in Brownian motion on a tilted periodic potential

E. Heinsalu, R. Tammelo, T. Örd *

Institute of Theoretical Physics, University of Tartu,
4 Tähe Str., 51010 Tartu, Estonia

Abstract

The paper studies the overdamped motion of Brownian particles in a tilted sawtooth potential. The dependencies of the diffusion coefficient and coherence level of Brownian transport on temperature, tilting force, and the shape of the potential are analyzed. It is demonstrated that at low temperatures the coherence level of Brownian transport stabilizes in the extensive domain of the tilting force where the value of the Péclet factor is $Pe = 2$. This domain coincides with the one where the enhancement of the diffusion coefficient *versus* the tilting force is the most rapid. The necessary and sufficient conditions for the non-monotonic behaviour of the diffusion coefficient as a function of temperature are found. The effect of the acceleration of diffusion by bias and temperature is demonstrated to be very sensitive to the value of the asymmetry parameter of the potential.

Key words: Diffusion; Coherence of Brownian transport; Tilted sawtooth potential
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In recent years the anomalous properties of thermal diffusion in tilted periodic potentials have been considered in a number of papers [1,2,3,4,5]. The effect of the giant amplification of diffusion by bias with respect to free diffusion was observed [2,3] and the non-monotonic behaviour of the diffusion coefficient as a function of temperature was found [4]. The influence of spatially modulated friction on diffusion and coherent transport in a tilted washboard potential was investigated in Ref. [5], and similar effects caused by spatially periodic temperature were discussed in Ref. [6].

* corresponding author
Email addresses: ehe@ut.ee (E. Heinsalu), teetord@ut.ee (T. Örd).

In the present contribution we study the diffusion and coherence of overdamped Brownian particles in a biased sawtooth potential in the space of the tilting force F, temperature T, and asymmetry parameter k of the potential. We ascertain the characteristic features of Brownian transport in the system under consideration and obtain the relevant conditions for non-monotonic dependence of the diffusion coefficient on temperature.

The equation of one-dimensional overdamped motion of a Brownian particle in dimensionless units reads

$$\frac{dx(t)}{dt} = -\frac{dV(x)}{dx} + \xi(t) \ , \tag{1}$$

where $V(x)$ is a tilted periodic potential and $\xi(t)$ is Gaussian white noise.

Applying the general approach developed in Refs. [2,3] to a piecewise linear potential of the period $L = 1$, we obtain by means of cumbersome calculations the following algebraic expressions for the current and diffusion coefficient ($0 < k < 1$, $k = 0.5$ corresponds to the symmetric potential; $F \geq 0$, while above the critical tilt, $F > F_{cr} = 1$, the potential has no local minima):

$$\langle \dot{x} \rangle = \frac{\varphi_0}{Z} \ , \quad D = \frac{TY}{Z^3} \ , \tag{2}$$

where

$$Z = \left(\frac{k}{a} - \frac{1-k}{b}\right)\varphi_0 + T\left(\frac{1}{a} + \frac{1}{b}\right)^2 \varphi_a\varphi_b \ , \tag{3}$$

$$\begin{aligned} Y = {} & \left(\frac{k}{a^3} - \frac{1-k}{b^3}\right)\varphi_0^3 + 3T\left(\frac{1}{a^3} + \frac{1}{b^3}\right)\left(\frac{1}{a} + \frac{1}{b}\right)\varphi_0^2\varphi_a\varphi_b \\ & + \frac{1}{2}T\left(\frac{1}{a} + \frac{1}{b}\right)^2 \varphi_0 \left[\frac{1}{a^2}\varphi_a^2\tilde{\varphi}_b - \frac{1}{b^2}\varphi_b^2\tilde{\varphi}_a\right] \\ & + 2\left(\frac{1}{a} + \frac{1}{b}\right)^2 \varphi_0 \left[\frac{k}{a}\varphi_a^2(1-\varphi_b) - \frac{1-k}{b}\varphi_b^2(1+\varphi_a)\right] \\ & + T\left(\frac{1}{a} + \frac{1}{b}\right)^3 \left[\frac{1}{a}\varphi_a^3\varphi_b(1-\varphi_b) + \frac{1}{b}\varphi_b^3\varphi_a(1+\varphi_a)\right] \ , \end{aligned} \tag{4}$$

with

$$a = \frac{1-(1-F)k}{(1-k)k} \ , \quad b = \frac{1-F}{1-k} \ , \tag{5}$$

$$\varphi_0 = 1 - \exp\left(-\frac{F}{T(1-k)}\right) \ , \tag{6}$$

$$\varphi_a = \exp\left(\frac{1-F}{T}\right) - 1 \ , \quad \varphi_b = 1 - \exp\left(-\frac{1-(1-F)k}{T(1-k)}\right) \ , \tag{7}$$

$$\tilde{\varphi}_a = \exp\left(\frac{2(1-F)}{T}\right) - 1 \ , \quad \tilde{\varphi}_b = 1 - \exp\left(-\frac{2[1-(1-F)k]}{T(1-k)}\right) \ . \tag{8}$$

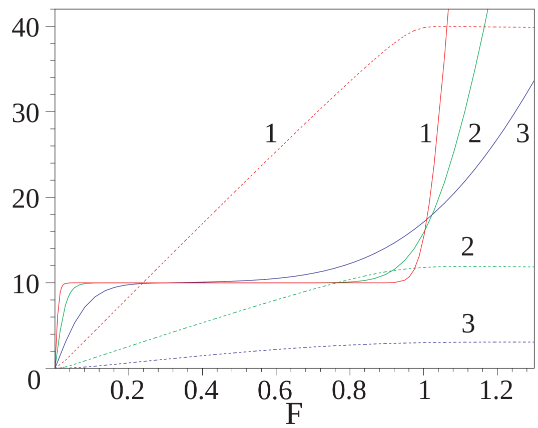

Fig. 1. Comparison of the dependencies of the Péclet factor and diffusion coefficient on the tilting force for various temperatures at fixed $k = 0.5$. Solid lines: $5 \times Pe$ *vs* F, dashed lines: $\log[D(F)/D(0)]$ *vs* F. Curves 1: $T = 0.01$, curves 2: $T = 0.03$, curves 3: $T = 0.09$.

A relevant quantity characterizing the coherence level of Brownian motion is the Péclet factor,

$$Pe = \frac{\langle \dot{x} \rangle}{D} = \frac{\varphi_0 Z^2}{TY} \ . \tag{9}$$

On the basis of the algebraic formulae obtained, we will analyze the behaviour of the diffusion coefficient and the Péclet factor in the space of the system parameters.

Firstly, we consider the correlation between the coherence level of Brownian transport and the acceleration of diffusion by the external tilting force. The comparative plot of D and Pe *versus* F is shown in Fig. 1. One can see that the function $Pe(F)$ has a point of inflection which turns into a wide plateau at low temperatures. For the values of F from zero up to the end of the plateau, the behaviour of $Pe(F)$ is described with great accuracy by the expression

$$Pe = 2 \tanh \frac{F}{2T(1-k)} \ , \tag{10}$$

which stems analytically from Eq. (9) in the proper approximation. We emphasize that in the same domain where $Pe = 2$, the increase of the diffusion coefficient caused by the tilt is the most rapid, following quite exactly the law $c^{\alpha_1 + \alpha_2 F}$ where c and $\alpha_{1,2}$ depend on T and k. Consequently, in the region of parameters, where the substantial acceleration of diffusion (and also current) occurs, the current and the diffusion are synchronized. Note also that the stabilization of the coherence level at the value of the Péclet factor $Pe = 2$ is a characteristic feature of the Poisson process [7] such as the Poisson enzymes in kinesin kinetics [8,9,10].

Now let us discuss the dependence of diffusion on the system parameters.

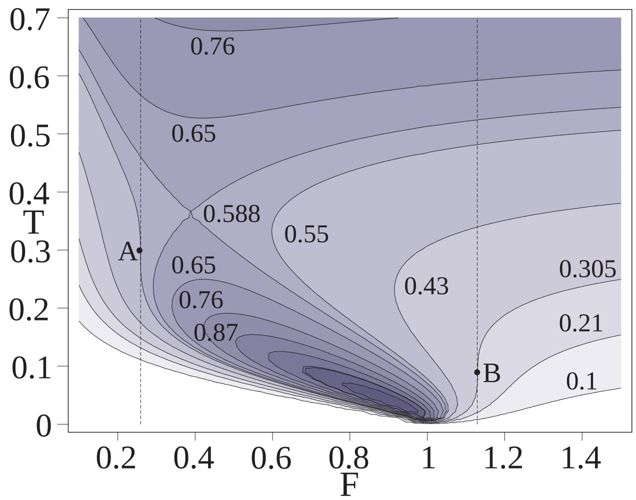

Fig. 2. Contourplot of the surface $D = D(T, F)$ for $k = 0.95$. The values of the diffusion coefficient $D(T, F) = \text{const}$ are displayed. To the maximum and saddle points of D correspond, respectively, the values $F_M \approx 0.9144$, $T_M \approx 0.0364, D_M \approx 1.3086$ and $F_S \approx 0.388, T_S \approx 0.363,\ D_S \approx 0.588$.

Figure 2 presents the analytic properties of the diffusion coefficient as a function of temperature and tilting force, displaying the contourplot of the surface $D = D(T, F)$. The surface exhibits two stationary points, a maximum and a saddle point, whose coordinates are given in the figure caption. The plot reflects fully the characteristic features of the non-monotonic behaviour of diffusion: (i) One can observe in Fig. 2 that the function $D(T)|_{F=\text{const}}$ has a maximum and a minimum if $F_A < F < F_B$. The maximum of $D(T)$ becomes rapidly narrower and higher as k approaches unity (see Fig. 3). For

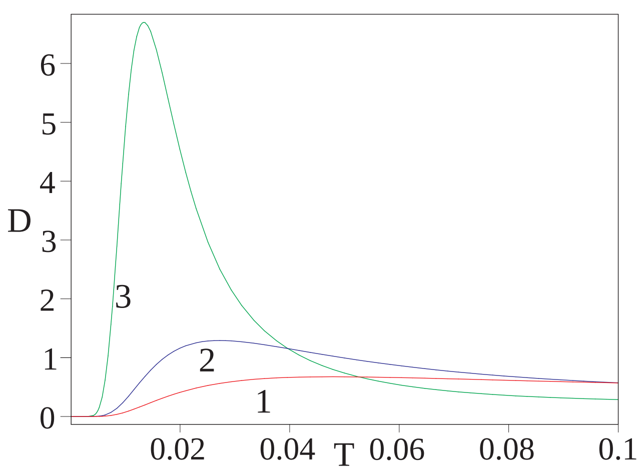

Fig. 3. The diffusion coefficient D *vs* temperature T at $F = 0.95$ for various values of the asymmetry parameter. Curve 1: $k = 0.9$, curve 2: $k = 0.95$, curve 3: $k = 0.99$.

$k < k_E \approx 0.8285$, the saddle point of the surface $D(T, F)$ disappears, while $D(T)|_{F=\text{const}}$ is a monotonic function of temperature, the latter property being independent of bias. There also exists a limiting tilting force $F_C \approx 1.1292$. If $F > F_C$, the dependence $D(T)|_{F=\text{const}}$ is monotonic for arbitrary k. The

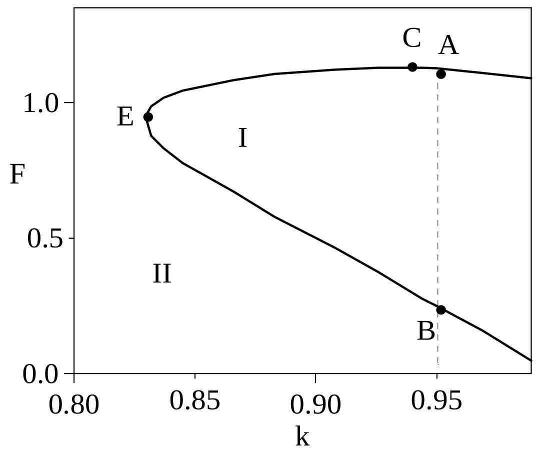

Fig. 4. The phase-diagram in the (F, k)-plane representing the regions corresponding to the different analytical properties of the diffusion coefficient as a function of temperature: the dependence $D(T)$ is non-monotonic in the region I, whereas it is monotonic in the region II.

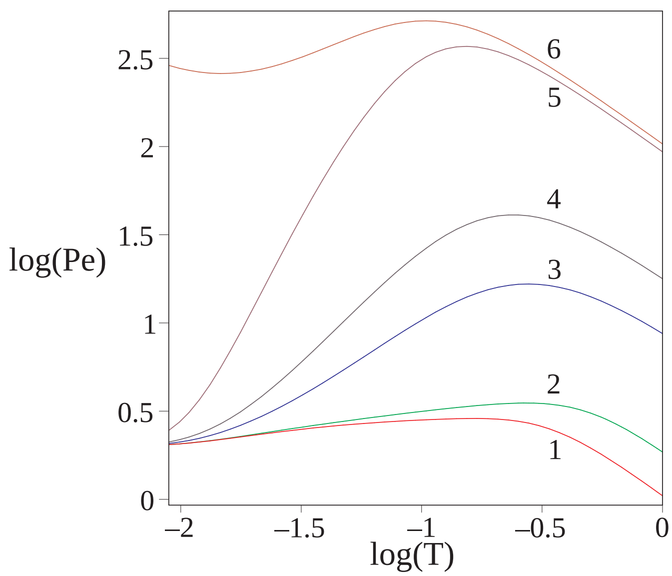

Fig. 5. The plot of the Péclet factor *vs* temperature for various values of the asymmetry parameter k of the potential at $F = 0.95$ (curves 1-5) and $F = 1.05$ (curve 6). Curve 1: $k = 0.1$, curve 2: $k = 0.5$, curve 3: $k = 0.9$, curve 4: $k = 0.95$, curves 5, 6: $k = 0.99$.

situation is summarized by the phase-diagram in Fig. 4. (ii) Contrary to the dependence $D(T)|_{F=\text{const}}$, the function $D(F)|_{T=\text{const}}$ always has a maximum, while the larger values of k are more favourable for the amplification of diffusion by bias.

The dependence of the Péclet factor on temperature for various values of k and F is depicted in Fig. 5. The curves $Pe(T)$ have a maximum, which occurs also for the values of the tilt slightly above the critical (curve 6). With a further increase of F, the maximum of $Pe(T)$ disappears. As it is seen in Fig. 5,

the optimal level of Brownian transport determined by the maximal value of the Péclet number is sensitive to the variation of the shape of the periodic potential: the optimal level rises with the increase of k. At the same time, if $k > k_E$, the dependence $D(T)$ can be non-monotonic (see Fig. 4). Then the larger values of k deepen the minimum of $D(T)$, which follows the maximum as temperature increases, enlarging by that the Péclet number. In this sense the situation is analogous to the results of Ref. [5] where the enhancement of the coherence of Brownian motion in a certain temperature range due to frictional inhomogeneity associates with the suppression of diffusion by the same factor.

To conclude, we emphasize that there exists a significant correlation between the acceleration of diffusion by tilting force and the stabilization of the coherence level of Brownian motion, resulting from the interplay of periodic potential, bias and white noise. It seems that this phenomenon is quite universal and manifests itself for arbitrary periodic potentials where initially strongly suppressed transport is enhanced by bias generating the considerable amplification of diffusion in comparison with free diffusion. One can expect that such a relationship reflects some intrinsic features of the interdependence of diffusion and current driven by external force.

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